

## SECTION 3. EQUILIBRIUM CONSTANTS

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#### 3.1 Format

Some of the three-body reactions in Table 2 form products that are thermally unstable at atmospheric temperatures. In such cases the thermal decomposition reaction may compete with other loss processes, such as photodissociation or radical attack. Table 3 lists the equilibrium constants, K(T), for several reactions which may fall into this category. The table has three column entries, the first two being the parameters A and B which can be used to express K(T):

$$K(T)/\text{cm}^3 \text{molecule}^{-1} = A \exp(B/T) \quad (200 < T < 300 \text{ K})$$

The third column entry in Table 3 is the calculated value of K at 298 K.

The data sources for K(T) are described in the individual notes to Table 3.

#### 3.2 Definitions

When values of the heats of formation and entropies of all species are known at the temperature T, we note that:

$$\log_{10} \left[ K(T) / \text{cm}^3 \text{molecule}^{-1} \right] = \frac{\Delta S^\circ_T}{2.303R} - \frac{\Delta H^\circ_T}{2.303RT} + \log_{10}(T) - 21.87$$

Where the superscript “o” refers to a standard state of one atmosphere. In some cases K values were calculated from this equation, using thermochemical data. In other cases the K values were calculated directly from kinetic data for the forward and reverse reactions. When available, JANAF values were used for the equilibrium constants. The following equations were then used to calculate the parameters A and B:

$$B/\text{°K} = 2.303 \left[ \frac{(300 \times 200)}{(300-200)} \right] \log_{10} \left( \frac{K_{200}}{K_{300}} \right) = 1382 \log_{10} \left( \frac{K_{200}}{K_{300}} \right)$$

$$\log_{10}(A) = \log_{10}(K(T)) - \frac{B}{2.303 T}$$

The relationships between the parameters A and B and the quantities  $\Delta S^\circ(298 \text{ K})$  and  $\Delta H^\circ(298 \text{ K})$  are:

$$A = \frac{eR'T}{N_{av}} \exp \left( \frac{\Delta S^\circ}{R} \right) = 3.7 \times 10^{-22} T \exp \left( \frac{\Delta S^\circ}{R} \right)$$

where  $R' = 82.1 \text{ cm}^3 \text{ atm mole}^{-1} \text{K}^{-1}$ , and  $N_{av} = 6.02 \times 10^{23} \text{ molecule mole}^{-1}$  and

$$B/\text{°K} = - \left[ \frac{\Delta H^\circ + RT}{R} \right]$$

Table 3-1. Equilibrium Constants

Reaction	A/cm <sup>3</sup> molecule <sup>-1</sup>	B/°K	K <sub>eq</sub> (298 K)	f(298 K) <sup>a</sup>	g	Note
HO + NO <sub>2</sub> → HOONO	3.9×10 <sup>-27</sup>	10125	2.2×10 <sup>-12</sup>	2	-400	<a href="#">1</a>
HO <sub>2</sub> + NO <sub>2</sub> → HO <sub>2</sub> NO <sub>2</sub>	2.1×10 <sup>-27</sup>	10900	1.6×10 <sup>-11</sup>	1.3	100	<a href="#">2</a>
NO + NO <sub>2</sub> → N <sub>2</sub> O <sub>3</sub>	3.3×10 <sup>-27</sup>	4667	2.1×10 <sup>-20</sup>	2	100	<a href="#">3</a>
NO <sub>2</sub> + NO <sub>2</sub> → N <sub>2</sub> O <sub>4</sub>	5.9×10 <sup>-29</sup>	6643	2.8×10 <sup>-19</sup>	1.4	100	<a href="#">4</a>
NO <sub>2</sub> + NO <sub>3</sub> → N <sub>2</sub> O <sub>5</sub>	2.7×10 <sup>-27</sup>	11000	2.9×10 <sup>-11</sup>	1.2	100	<a href="#">5</a>
CH <sub>3</sub> O <sub>2</sub> + NO <sub>2</sub> → 3CH <sub>3</sub> O <sub>2</sub> NO <sub>2</sub>	9.5×10 <sup>-29</sup>	11234	2.2×10 <sup>-12</sup>	1.3	500	<a href="#">6</a>
CH <sub>3</sub> C(O)O <sub>2</sub> + NO <sub>2</sub> → CH <sub>3</sub> C(O)O <sub>2</sub> NO <sub>2</sub>	9.0×10 <sup>-29</sup>	14000	2.3×10 <sup>-8</sup>	1.2	200	<a href="#">7</a>
CH <sub>3</sub> CH <sub>2</sub> C(O)O <sub>2</sub> + NO <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> C(O)O <sub>2</sub> NO <sub>2</sub>	9.0×10 <sup>-29</sup>	14000	2.3×10 <sup>-8</sup>	10	800	<a href="#">8</a>
CH <sub>3</sub> C(O)CH <sub>2</sub> + O <sub>2</sub> → CH <sub>3</sub> C(O)CH <sub>2</sub> O <sub>2</sub>	7×10 <sup>-27</sup>	13000	6×10 <sup>-8</sup>	10	800	<a href="#">9</a>
F + O <sub>2</sub> → FOO	4.5×10 <sup>-25</sup>	6118	3.7×10 <sup>-16</sup>	1.5	300	<a href="#">10</a>
Cl + O <sub>2</sub> → ClOO	6.6×10 <sup>-25</sup>	2502	2.9×10 <sup>-21</sup>	1.7	100	<a href="#">11</a>
Cl + CO → ClCO	3.5×10 <sup>-25</sup>	3730	9.6×10 <sup>-20</sup>	1.2	200	<a href="#">12</a>
ClO + O <sub>2</sub> → ClO O <sub>2</sub>	2.9×10 <sup>-26</sup>	<3700	<7.2×10 <sup>-21</sup>			<a href="#">13</a>
ClO + ClO → Cl <sub>2</sub> O <sub>2</sub>	9.3×10 <sup>-28</sup>	8835	7.0×10 <sup>-15</sup>	1.2	300	<a href="#">14</a>
ClO + OCLO → Cl <sub>2</sub> O <sub>3</sub>	1.6×10 <sup>-27</sup>	7155	4.3×10 <sup>-17</sup>	1.3	300	<a href="#">15</a>
OCLO + NO <sub>3</sub> → O <sub>2</sub> ClONO <sub>2</sub>	6.6×10 <sup>-29</sup>	3971	4.0×10 <sup>-23</sup>	5.5	500	<a href="#">16</a>
OH + CS <sub>2</sub> → CS <sub>2</sub> OH	4.5×10 <sup>-25</sup>	5140	1.4×10 <sup>-17</sup>	1.4	300	<a href="#">17</a>
CH <sub>3</sub> S + O <sub>2</sub> → CH <sub>3</sub> SO <sub>2</sub>	1.8×10 <sup>-27</sup>	5545	2.2×10 <sup>-19</sup>	1.4	300	<a href="#">18</a>
Cl + CS <sub>2</sub> → Cl---CS <sub>2</sub>	1.8×10 <sup>-25</sup>	4982	3.3×10 <sup>-18</sup>	1.3	150	<a href="#">19</a>
Br+CH <sub>3</sub> SCH <sub>3</sub> →Br---(CH <sub>3</sub> ) <sub>2</sub> S	3.4×10 <sup>-25</sup>	3021	4.6×10 <sup>-15</sup>	1.2	100	<a href="#">20</a>

K/cm<sup>3</sup> molecule<sup>-1</sup> = A exp (B/T) [200 < T/K < 300] – shaded areas indicate changes or additions since JPL02-25

a f(298 K) is the uncertainty factor at 298 K, and g is a measure of the uncertainty in the quantity B. To calculate the uncertainty at temperatures other than 298 K, use the expression:

$$f(T) = f(298 \text{ K}) \exp \left[ g \left( \frac{1}{T} - \frac{1}{298} \right) \right]$$

### 3.3 Notes to Table 3

JPL Publication numbers for the most recent revision of the table entry and note are given at the end of each note.

1. HO + NO<sub>2</sub>. This value is for the HOONO product channel. Using the data from Hippler et al. [37], Golden et al. [30] performed a third law analysis using structures and frequencies from an ab initio quantum calculation at the QCISD(T)/cc-pVDZ level to extract the heat of formation of cis-cis HOONO at 0K of -9.28 kJ mol<sup>-1</sup>. The value at 298K is -15.7 kJ mole<sup>-1</sup>. (A small error in the entropy of HOONO caused Golden et al. [29] to suggest -8.60 kJ mole<sup>-1</sup>.) The data covers 430<T/K<475 with 30% uncertainties. The error limits reflect the fact that the uncertainty is greater at 298 K than in the temperature range where the data were taken. NEW ENTRY [Back to table](#)
2. HO<sub>2</sub> + NO<sub>2</sub>. The value was obtained by combining the expression from Table 2-1 for the rate constant of the reaction as written with that from an average of the expressions from Graham et al. [33] and Zabel [72] for the reverse reaction. Values for the entropy and heat of formation of pernitric acid may be extracted. These values are: S(298 K) = 71.7 cal mole<sup>-1</sup> K<sup>-1</sup> and ΔH<sub>f</sub>(298 K) = -12.9 kcal mole<sup>-1</sup>. If the entropy is calculated from the frequencies and moments of inertia given by Chen and Hamilton [16], the value becomes 71.0 and the heat is -13.1. The values in the Appendix to this report reflect these results. A study of the thermal decomposition of HO<sub>2</sub>NO<sub>2</sub> by Gierczak et al. [27] combined with values for the association reaction are in agreement. (Table: JPL06, Note: JPL06) [Back to table](#)
3. NO + NO<sub>2</sub>. The data are from JANAF [41] and Chao et al. [14]. This process is included because a measurement of the rate constant by Smith and Yarwood [63] and Markwalder et al. [44] shows that it is too slow to be an important process in most atmospheric and laboratory systems. (Table: 94-26, Note: 94-26) [Back to table](#)
4. NO<sub>2</sub> + NO<sub>2</sub>. The data are from JANAF [41] and Vosper [68], Chao et al. [15] and Amoruso et al. [1]. Rate data for this process are reported by Brunning et al. [7], Borrell et al. [4] Gozel et al. [31] and Markwalder et al. [44]. A direct study by Harwood and Jones [35] at low temperatures is in agreement with the recommendation. Re-evaluation of the data suggests slightly different error limits than recommended in JPL 02-25. Estupiñán et al. [23], Wollenhaupt and Crowley [71] and Tuchler et al. [65] deduce values that are in essential agreement, within uncertainties, with the recommendation. (Table: 02-25, Note: 02-25) [Back to table](#)
5. NO<sub>2</sub> + NO<sub>3</sub>. The recommendation is from Cantrell et al. [12]. They report rate constants for the decomposition reaction, which they combine with the rate constants of Orlando et al. [53] to obtain the equilibrium constant. Agreement is quite good with the data of Burrows et al. [9] and Cantrell et al. [11] and the room temperature data of Tuazon et al. [64] Perner et al. [56] and Hjorth et al. [38]. An evaluation by Pritchard [59] is also in excellent agreement with the recommendation. Pritchard [59] examined the data of Cantrell et al. [11], Burrows et al. [9], Graham and Johnston [32], Wangberg et al [69], Schott and Davidson [60], and the room temperature data of Tuazon et al. [64], Perner et al. [56] and Hjorth et al. [38]. He also included the values given by Smith et al. [62], and Kircher et al. [42], who combined data on the forward reaction, tabulated in Table 2-1, with decomposition data of Connell and Johnston [18] and Viggiano et al. [67]. The Pritchard [59] result was used as the basis for the value in JPL 00-3, but some uncertainties in the entropies of NO<sub>3</sub> and N<sub>2</sub>O<sub>5</sub> justify the reversion to the JPL 97-4 recommendations. In JPL 02-25, the values of the parameters were inadvertently left unchanged from those in JPL 00-3. The differences are very small. The one sigma error limits are better described with f(298) = 1.2. (Table: JPL06, Note: JPL06) [Back to table](#)
6. CH<sub>3</sub>O<sub>2</sub> + NO<sub>2</sub>. Zabel et al. [73] have measured k(dissociation) as a function of pressure (10<P/torr<800) and temperature (253<T/K<272). Bahta et al. [3] have measured k(dissociation) at 263 K. Using the values of k(recombination) suggested in this evaluation, (Table-2) Golden [28] has re-evaluated the equilibrium constant. Bridier et al. [6] measure an equilibrium constant in good agreement with this recommendation, reducing the uncertainty even further. (Table: JPL06, Note: JPL06) [Back to table](#)

7.  $\text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO}_2$ . The recommendation is derived from measurements of the rate constants in both directions by Bridier et al. [5]. These authors used the values of the rate constants at 298K and a calculated value of the entropy change to get a third law value of the equilibrium constant. Their value of the enthalpy is exactly reproduced in a theoretical study by Miller et al. [46]. (Table: JPL06, Note: JPL06) [Back to table](#)
8.  $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O}_2 + \text{NO}_2$ . Assumed to be the same as for PAN (Note 7). Both sides of the reaction differ from PAN by the group C-(C)(CO)(H)<sub>2</sub>. Error limits are estimated and expanded from those for PAN. (Table: 02-25, Note: 02-25) [Back to table](#)
9.  $\text{CH}_3\text{C}(\text{O})\text{CH}_2 + \text{O}_2$ . Estimated values of the entropy and enthalpy changes for the reaction are:  $\Delta S = -33$  e.u. and  $\Delta H = -26$  kcal/mole. The entropy is from group additivity and the enthalpy from group additivity for the hydroperoxide followed by assuming that the O-H bond dissociation energy is 88 kcal/mole. Error limits are estimated from the uncertainties in this procedure. (Table: 02-25, Note: 02-25) [Back to table](#)
10.  $\text{F} + \text{O}_2$ . Taken from Campuzano-Jost et al. [10]. There is good agreement with data from Pagsberg et al. [54]. This corresponds to a value for  $\Delta H_{f,298}(\text{FO}_2) = 6.13 \pm 0.5$  kcal mol<sup>-1</sup>. There are several modern theoretical computations [21, 24, 25] of this value, ranging from 6 to 9 kcal mol<sup>-1</sup>. (Table: JPL06, Note: JPL06) [Back to table](#)
11.  $\text{Cl} + \text{O}_2$ . Data are from Baer et al. [2], Nicovich et al. [50] and Mauldin et al. [45]. Zhu and Lin [75] have reported structure and frequency calculations and a heat of formation for ClOO. Using known thermochemistry for Cl and O<sub>2</sub> and entropy values for ClOO computed from,  $\Delta H_{f,0}$  (ClOO) =  $23.85 \pm 0.1$  kcal mole<sup>-1</sup> is obtained by the third law method from the individual data points of the Nicovich et al. [50] data. The Baer et al. [2] paper reports only one value at each temperature and only graphically, but yields essentially the same value as Nicovich et al [50]. The third law value from Mauldin et al. [45] is less stable by 0.4 kcal mole<sup>-1</sup>. Earlier values, both experimental and theoretical, of the structural parameters of ClOO are referenced in [75].  $S^\circ_{298}$  (ClOO) =  $64.6$  cal mole<sup>-1</sup> K<sup>-1</sup> and  $\Delta H_{f,298}$  (ClOO) =  $23.5 \pm 0.5$  kcal mole<sup>-1</sup> are recommended. (Table: JPL06, Note: JPL06) [Back to table](#)
12.  $\text{Cl} + \text{CO}$ . From fitting the data of Nicovich et al. [51] who measured both k and K between 185 and 260 K in N<sub>2</sub>. They report  $\Delta H_{f,298}$  (ClCO) =  $-5.2 \pm 0.6$  kcal mole<sup>-1</sup>. (Table: JPL06, Note: JPL06) [Back to table](#)
13.  $\text{ClO} + \text{O}_2$ . DeMore [20] reports  $K < 4 \times 10^{-18}$  cm<sup>3</sup> molecule<sup>-1</sup> at 197 K. His temperature dependence of the equilibrium constant is estimated using  $S^\circ_{298}$  (ClO·O<sub>2</sub>) =  $73$  cal mol<sup>-1</sup> K<sup>-1</sup> and  $\Delta H^\circ_{298} < 7.7$  kcal mol<sup>-1</sup>. A higher value of K has been proposed by Prasad [57], but it requires  $S^\circ$ (ClO·O<sub>2</sub>) to be about  $83$  cal mol<sup>-1</sup> K<sup>-1</sup>, which seems unreasonably high. Carter and Andrews [13] found no experimental evidence for ClO·O<sub>2</sub> in matrix experiments. Prasad and Lee [58] discuss these issues and question the validity of the upper limit reported by DeMore. (Table: 92-20, Note: 94-26) [Back to table](#)
14.  $\text{ClO} + \text{ClO}$ . The value is from a third-law calculation based on the data from Cox and Hayman [19] (except for the two lowest temperature points) and Nickolaisen et al.[49]. The entropy of ClOOCl, the value of which is  $71.9$  cal mol<sup>-1</sup> K<sup>-1</sup> at 300 K, is calculated from structures and frequencies calculated by Zhu and Lin [74]. The heat of formation at 300 K is  $\Delta H^\circ_{f,300} = 30.4$  kcal mol<sup>-1</sup>. A study of branching ratios of ClO + ClO channels in Cl<sub>2</sub>/O<sub>2</sub>/O<sub>3</sub> mixtures by Horowitz et al. [39] also finds the equilibrium constant in O<sub>2</sub> at 285 K to be in agreement with the recommendation. Avallone and Toohey used  $K = 1.99E-30\text{Exp}(8854/T)$  derived from *in situ* experiments. (Table: JPL06, Note: JPL06) [Back to table](#)
15.  $\text{ClO} + \text{OCIO}$ . Data are from Burkholder et al. [8], Hayman and Cox [36] and Green et al. [34]. The best van't Hoff fit to all the data (except for the lowest temperature point of) yields  $K/\text{cm}^3$  molecule<sup>-1</sup> =  $2.5 \times 10^{-25}\text{Exp}(5850/T)$  for {232< T/K<298}. A calculation of the entropy and heat capacity from the structure and frequencies of ClOCl(O)O reported by Zhu and Lin [76] allows a "3<sup>rd</sup> Law" fit that yields the recommended parameters. The 95% error limits encompass all the data. From the 3<sup>rd</sup> Law calculations  $S^\circ_{298}$  (Cl<sub>2</sub>O<sub>3</sub>)= $78.7$  cal mol<sup>-1</sup> K<sup>-1</sup> and  $\Delta H_{f,0}(\text{Cl}_2\text{O}_3) = 33.6$  kcal mol<sup>-1</sup> and  $\Delta H_{f,298}(\text{Cl}_2\text{O}_3) = 32.4$  kcal mol<sup>-1</sup>. (This compares to a calculated value of  $\Delta H_{f,0}(\text{Cl}_2\text{O}_3) = 32.3$  from [76] and 32.9 from a theoretical calculation by Sicre and Cobos [61]. Burkholder et al. [8] claim that treating the lowest vibration as a free internal rotation increases the entropy of ClOCl(O)O by almost 9 cal mol<sup>-1</sup> K<sup>-1</sup>. This value, repeated by Green et al. [34], is not correct. Clark and Francisco [17] calculated structure and frequencies and conclude that  $S^\circ_{298}$  (Cl<sub>2</sub>O<sub>3</sub>)= $78.5$  cal mol<sup>-1</sup> K<sup>-1</sup> in close agreement with the above, but they conclude that  $\Delta H_{f,0}(\text{Cl}_2\text{O}_3) = 36.9$  kcal mol<sup>-1</sup> by fitting the data of [8] and [36] including the lowest temperature point. Li et al. [43] have also reported theoretical calculations for

ClOCl(O)O. Their structure and frequencies are in general agreement with [76] and [17], but their energetics are quite different. (Table: JPL06, Note: JPL06) [Back to table](#)

16. OCIO + NO3. Theoretical calculations of Parthiban et al. [55]. This value replaces the value in 02-25 that was deduced by Friedl et al. [26]. Uncertainties are based on  $\pm 1$  kcal mole $^{-1}$  uncertainty in calculated heat of formation. (Table: JPL06, Note: JPL06) [Back to table](#)
17. OH + CS2. Fit to the data of Murrells et al. [47], Hynes et al. [40] and Diau and Lee [22] between 246 and 318 K. Re-analysis of errors led to lower value of g than in JPL-02-25. (Table: JPL06, Note: JPL06) [Back to table](#)
18. CH3S + O2. Turnipseed et al. [66] report the equilibrium constant for  $216 \leq T/K \leq 258$ . From a third law analysis using  $\Delta S^\circ_{237} = -36.8 \pm 2.6$  eu, they obtain  $\Delta H^\circ_{237} = -11.5 \pm 0.9$  kcal/mole. (Table: 94-26, Note: 94-26) [Back to table](#)
19. Cl + CS2. Fit to the data of Nicovich et al. [52] between 193 and 258 K. NEW ENTRY [Back to table](#)
20. Br + CH3SCH3. Second Law fit to data of Wine et al. [70] and Nakano et al. [48]. This corresponds to a bond dissociation energy in the adduct of 13.84 kcal mole $^{-1}$ . NEW ENTRY [Back to table](#)

### 3.4 References

1. Amoruso, A., L. Crescentini, G. Fiocco and M. Volpe, 1993, *J. Geophys. Res.*, 98, 16857-16863.
2. Baer, S., H. Hippler, R. Rahn, M. Siefke, N. Seitzinger and J. Troe, 1991, *J. Chem. Phys.*, 95, 6463-6470.
3. Bahta, A., R. Simonaitis and J. Heicklen, 1982, *J. Phys. Chem.*, 86, 1849.
4. Borrell, P., C. J. Cobos and K. Luther, 1988, *J. Phys. Chem.*, 92, 4377-4384.
5. Bridier, I., F. Caralp, H. Loirat, R. Lesclaux, B. Veyret, K. H. Becker, A. Reimer and F. Zabel, 1991, *J. Phys. Chem.*, 95, 3594-3600.
6. Bridier, I., R. Lesclaux and B. Veyret, 1992, *Chem. Phys. Lett.*, 191, 259-263.
7. Brunning, J., M. J. Frost and I. W. M. Smith, 1988, *Int. J. Chem. Kinetics*, 20, 957.
8. Burkholder, J. B., R. L. Mauldin, R. J. Yokelson, S. Solomon and A. R. Ravishankara, 1993, *J. Phys. Chem.*, 97, 7597-7605.
9. Burrows, J. P., G. S. Tyndall and G. K. Moortgat, 1985, *Chem. Phys. Lett.*, 119, 193-198.
10. Campuzano-Jost, P., A. E. Croce, H. Hippler, M. Siefke, and J. Troe, 1995, *J. Chem. Phys.*, 102, 5317-5326.
11. Cantrell, C. A., J. A. Davidson, A. H. McDaniel, R. E. Shetter and J. G. Calvert, 1988, *J. Chem. Phys.*, 88, 4997-5006.
12. Cantrell, C. A., R. E. Shetter, J. G. Calvert, G. S. Tyndall and J. J. Orlando, 1993, *J. Phys. Chem.*, 97, 9141-9148.
13. Carter, R. O. and L. Andrews, 1981, *J. Phys. Chem.*, 85, 2351.
14. Chao, J., R. C. Wilhoit and B. J. Zwolinski, 1974, *Thermochim. Acta*, 10, 359-360.
15. Chao, J., R. C. Wilhoit and B. J. Zwolinski, 1974, *Thermochim. Acta*, 10, 361-371.
16. Chen, Z. and T. P. Hamilton, 1996, *J. Phys. Chem.*, 100, 15731-15734.
17. Clark, J. and J. S. Francisco, 1997, *J. Phys. Chem. A*, 101, 7145-7153.
18. Connell, P. S. and H. S. Johnston, 1979, *Geophys. Res. Lett.*, 6, 553-556.
19. Cox, R. A. and G. D. Hayman, 1988, *Nature*, 332, 796-800.
20. DeMore, W. B., 1990, *Geophys. Res. Lett.*, 17, 2353-2355.
21. Denis, P. A., and O. N. Ventura, 2004, *Chem. Phys. Lett.*, 385, 292-297.
22. Diau, E. W.-G. and Y.-P. Lee, 1991, *J. Phys. Chem.*, 95, 7726-7732.
23. Estupiñán, E. G., J. M. Nicovich and P. H. Wine, 2001, *J. Phys. Chem. A*, 105, 9697-9703.
24. Feller, D. and D. A. Dixon, 2003, *J. Phys. Chem. A*, 107, 9641-9651.
25. Francisco, J. S., Y. Zhao, W. A. Lester, Jr., and I. H. Williams, 1992, *J. Chem. Phys.*, 96, 2861-2867.
26. Friedl, R. R., S. P. Sander and Y. L. Yung, 1992, *J. Phys. Chem.*, 96, 7490-7493.
27. Gierczak, T., E. Jimenez, V. Riffault, J. B. Burkholder, and A. R. Ravishankara, 2005, *J. Phys. Chem. A*, 109, 586-596.
28. Golden, D. M., 2005, *Int. J. Chem. Kinet.*, Accepted.
29. Golden, D. M., J. R. Barker and L. L. Lohr, 2004, *J. Phys. Chem. A*, 108, 8552.
30. Golden, D. M., J. R. Barker, and L. L. Lohr, 2003, *J. Phys. Chem. A*, 107, 11057-11071.
31. Gozel, P., B. Calpani and H. van den Bergh, 1984, *Isrl. J. Chem.*, 24, 210.
32. Graham, R. A. and H. S. Johnston, 1978, *J. Phys. Chem.*, 82, 254-268.
33. Graham, R. A., A. M. Winer and J. N. Pitts, Jr., 1977, *Chem. Phys. Lett.*, 51, 215.
34. Green, T. J., M. Islam, P. Guest, K. Hickson, C. E. Canosa-Mas, and R. P. Wayne, 2003, *Phys. Chem. Chem. Phys.*, 5, 5409-5418.
35. Harwood, M. H. and R. L. Jones, 1994, *J. Geophys. Res.*, 99, 22955-22964.
36. Hayman, G. D. and R. A. Cox, 1989, *Chem. Phys. Lett.*, 155, 1-7.
37. Hippler, H., S. Nasterlack and F. Striebel, 2002, *Phys. Chem. Chem. Phys.*, 4, 2959-2964.
38. Hjorth, J., J. Notholt and G. Restelli, 1992, *Int. J. Chem. Kinet.*, 24, 51-65.
39. Horowitz, A., J. N. Crowley and G. K. Moortgat, 1994, *J. Phys. Chem.*, 98, 11924-11930.
40. Hynes, A. J., P. H. Wine and J. M. Nicovich, 1988, *J. Phys. Chem.*, 92, 3846-3852.
41. JANAF *Thermochemical Tables*, Third ed.; National Bureau of Standards, 1985.
42. Kircher, C. C., J. J. Margitan and S. P. Sander, 1984, *J. Phys. Chem.*, 88, 4370-4375.
43. Li, Q., S. Lu, Y. Xie, P. V. R. Schleyer and H. F. Schaefer, III, 2003, *Int. J. Quantum Chem.*, 95, 731-757.
44. Markwalder, B., P. Gozel and H. van den Bergh, 1992, *J. Chem. Phys.*, 97, 5472-5479.
45. Mauldin, R. L., III, J. B. Burkholder and A. R. Ravishankara, 1992, *J. Phys. Chem.*, 96, 2582-2588.
46. Miller, C. E., J. I. Lynton, D. M. Keevil and J. S. Franscisco, 1999, *J. Phys. Chem. A*, 103, 11451-11459.
47. Murrells, T. P., E. R. Lovejoy and A. R. Ravishankara, 1990, *J. Phys. Chem.*, 94, 2381-2386.

48. Nakano, Y., M. Goto, S. Hashimoto, M. Kawasaki, and T. J. Wallington, 2001, *J. Phys. Chem. A*, 105, 11045-11050.
49. Nickolaisen, S. L., R. R. Friedl and S. P. Sander, 1994, *J. Phys. Chem.*, 98, 155-169.
50. Nicovich, J. M., K. D. Kreutter, C. J. Shackelford and P. H. Wine, 1991, *Chem. Phys. Lett.*, 179, 367-373.
51. Nicovich, J. M., K. D. Kreutter and P. H. Wine, 1990, *J. Chem. Phys.*, 92, 3539-3544.
52. Nicovich, J. M. and P. H. Wine, 1990, *Int. J. Chem. Kinet.*, 22, 379-397.
53. Orlando, J. J., G. S. Tyndall, C. A. Cantrell and J. G. Calvert, 1991, *J. Chem. Soc. Far. Trans.*, 87, 2345-2349.
54. Pagsberg, P. B., E. Ratajczak, A. Sillesen and J. T. Jodkowski, 1987, *Chem. Phys. Lett.*, 141, 88-94.
55. Parthiban, S., T. J. Lee, S. Guha, and J. S. Francisco, 2003, *J. Amer. Chem. Soc.*, 125, 10446-10458.
56. Perner, D., A. Schmeltekopf, R. H. Winkler, H. S. Johnston, J. G. Calvert, C. A. Cantrell and W. R. Stockwell, 1985, *J. Geophys. Res.*, 90, 3807-3812.
57. Prasad, S. S., 1980, *Nature*, 285, 152.
58. Prasad, S. S. and T. J. Lee, 1994, *J. Geophys. Res.*, 99, 8225-8230.
59. Pritchard, H. O., 1994, *Int. J. Chem. Kinet.*, 26, 61-72.
60. Schott, G. and N. Davidson, 1958, *J. Amer. Chem. Soc.*, 80, 1841-1853.
61. Sicre, J. E. a. C. J. C., 2003, *J. Molec. Structure*, 620, 215-226.
62. Smith, C. A., A. R. Ravishankara and P. H. Wine, 1985, *J. Phys. Chem.*, 89, 1423-1427.
63. Smith, I. W. M. and G. Yarwood, 1986, *Chem. Phys. Lett.*, 130, 24-28.
64. Tuazon, E. C., E. Sanhueza, R. Atkinson, W. P. L. Carter, A. M. Winer and J. N. Pitts, Jr., 1984, *J. Phys. Chem.*, 88, 3095-3098.
65. Tuchler, M. F., K. L. Schmidt, and M. Morgan, 2005, *Chem. Phys. Lett.*, 401, 393-399.
66. Turnipseed, A. A., S. B. Baron and A. R. Ravishankara, 1992, *J. Phys. Chem.*, 96, 7502-7505.
67. Viggiano, A. A., J. A. Davidson, F. C. Fehsenfeld and E. E. Ferguson, 1981, *J. Chem. Phys.*, 74, 6113-6125.
68. Vosper, A. J., 1970, *J. Chem. Soc. A*, 1970, 625.
69. Wangberg, I., T. Etzkorn, I. Barnes, U. Platt and K. H. Becker, 1997, *J. Phys. Chem. A*, 101, 9694-9698.
70. Wine, P. H., J. M. Nicovich, R. E. Stickel, Z. Zhao, C. J. Shackelford, K. D. Kreutter, E. P. Daykin and S. Wang *The Tropospheric Chemistry of Ozone in the Polar Regions*; Springer-Verlag: Berlin, 1993; Vol. 17.
71. Wollenhaupt, M. and J. N. Crowley, 2000, *J. Phys. Chem. A*, 104, 6429-6438.
72. Zabel, F., 1995, *Zeitschrift fur Physikalische Chemie*, 188, 119-142.
73. Zabel, F., A. Reimer, K. H. Becker and E. H. Fink, 1989, *J. Phys. Chem.*, 93, 5500-5507.
74. Zhu, R. S., and M. C. Lin, 2003, *J. Chem. Phys.*, 118, 4094-4106.
75. Zhu, R. S. and M. C. Lin, 2003, *J. Chem. Phys.*, 119, 2075-2082.
76. Zhu, R. S. and M. C. Lin, 2003, *J. Chem. Phys.*, 118, 8645-8655.